Calculation of transport coefficients of air-water vapor mixtures thermal plasmas used in circuit breakers

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Abstract: In this paper we calculate the transport coefficients of plasmas formed by air and water vapor mixtures. The calculation, which assume local thermodynamic equilibrium (LTE) are performed in the temperature range from 500 to 12000 K. We use the Gibbs free energy minimization method to determine the equilibrium composition of the plasmas, which is necessary to calculate the transport coefficients. We use the Chapman-Enskog method to calculate the transport coefficients. The results are presented and discussed according to the rate of water vapor. The results of the total thermal conductivity and electrical conductivity show in particular that the increasing of the rate of water vapor in air can be interesting for power cut. This could be improve the performance of plasma during current breaking in air contaminate by the water vapor.

Keywords: **Plasma, Equilibrium composition, Transport coefficients**.

1) Introduction

The current cut in the circuit breakers is obtained by separating electrodes in air or in compressed air [1, 2].When a short-circuit or an overload appears in the electrical circuit, the contacts of the circuit breaker separate and generates an electric arc [1-3] which interacts with the surrounding gas and creates a plasma of this gas [1, 2]. Other studies on the electrical arc had shown the influence of the insulator vapor [1, 5-8], metal of contacts [1, 9-11] and hydrogen atom [1, 2, 5, 8] on the engendered plasmas characteristics. In this paper, we are interested by the influence of hydrogen on plasma characteristics for electrical current breaking. This hydrogen can be brought by water vapor in the air. The knowledge of transport coefficients is fundamental to evaluate and compare the performance of plasmas for current breaking [5] and also, transport coefficients are the indispensable data for modeling of electric plasmas arcs [12-14].We undertake in this study the calculation of the transport coefficients of air-water vapor mixtures thermal plasmas. This mixture can be naturally formed because of air humidity [1, 2], but the percentage of water vapor in the atmospheric air is limited. In the zones with great humidity, we can have a maximum percentage of water vapor in air around 7% at a temperature of 40°C [1, 2]. As this value is not sufficient to bring enough hydrogen for better performances, we choose to study air-water vapor mixtures with often high water vapor percentage. The plasmas considered are: 95% air - 5% water vapor; 90% air - 10% water vapor, 50% air - 50% water vapor and 20% air - 80% water vapor. These four mixtures are chosen to determine the water vapor influence on the plasmas transport coefficients. The

increase of water vapor in the mixture could be done during the breaking of the electric current by water injection. Assuming local thermodynamic equilibrium (LTE), calculations are made in a temperatures range from 500 K to 12000 K. We suppose that the air is constituted of 80% nitrogen (N_2) and 20% oxygen (O_2). In the figures 1, 2 and 3, we compare our results of dry air plasma with those of P. Fauchais and al. Then, we present and discuss our results of transport coefficients of plasma formed of air-water vapor mixture. This study completes the one of Kagoné and al [1] to have a database on the range of temperatures from 500 K to 30000 K for the modeling of plasma formed by air- water vapor mixtures.

2) Transport coefficients

The initial step in the calculation of transport coefficients is the determination of the equilibrium composition of the plasma. This is done by using the widely known method based on the Gibbs free energy minimization [12, 14, 16]. For air-water vapor mixture, we take into account 11 monatomic species: H, H^-, H^+, N, N^+,N^{++},O, O^-, O^+, O^{++} , and electrons; 18 diatomic species: H_2, H_2^-, H_2^+, N_2, N_2^-, N_2^+, NH, NH^-, NH^+, NO, NO^-, NO^+, O_2, O_2^-, O_2^+, OH, OH^-, OH^+, and 11 polyatomic species: O_3, H_2O, N_2O, NH_3, N_2O_3, HNO_2, HO_2, N_2O_4, H_2N_2, N_2O_5, HNO_3. The monatomic and diatomic specific thermodynamic properties such as enthalpies, chemical potentials are calculated by the fitting coefficients found in [15]. For polyatomic chemical species their specific thermodynamic properties are obtained in Janaf tables [17].

The transport coefficients were calculated using the Chapman-Enskog method based on sonine polynomials development [1, 5, 12, 13, 18-22]. In our study we considered thermal conductivity, electrical conductivity and dynamical viscosity of the plasma.

2.1) Thermal conductivity coefficient

The total thermal conductivity λ_{tot} can be separated into four terms with a good accuracy [1,14]:

$$\lambda_{tot} = \lambda_{tr}^e + \lambda_{tr}^h + \lambda_{int} + \lambda_{react} \qquad (1)$$

Where λ_{tr}^e is the translational thermal conductivity of electrons, λ_{tr}^h the translational thermal conductivity of heavy species particles, λ_{int} the internal thermal conductivity and λ_{react} the chemical reaction thermal conductivity. Thermal conductivity of electrons at the third approximation order is given by [1, 14]:

$$\lambda_{tr}^e = \frac{75}{8} k\, n_1^2 \sqrt{\frac{2\pi RT}{m_1}} \frac{q^{22}}{q^{11}q^{22}-\left(q^{12}\right)^2} \qquad (2)$$

The translational thermal conductivity due to the heavy species in the second order approximation can be written as [23]:

$$\lambda_{tr}^h = 4 \frac{\begin{vmatrix} L_{11} & \dots & L_{1\mu} & X_1 \\ \dots & L_{ii} & \dots & \dots \\ L_{\mu 1} & \dots & L_{\mu\mu} & X_\mu \\ X_1 & \dots & X_\mu & 0 \end{vmatrix}}{\begin{vmatrix} L_{11} & \dots & L_{1\mu} \\ \dots & L_{ii} & \dots \\ L_{\mu 1} & \dots & L_{\mu\mu} \end{vmatrix}} \quad (3)$$

The coefficients L_{ij} are given by Muckenfuss [13, 23]. The internal conductivity due to the effect of internal degrees of freedom is taken into account with the Eucken correction [14]. The first order in approximation of Chapman-Enskog's method [13] given by:

$$\lambda_{int} = \sum_{i=2}^{\mu} \frac{\frac{PD_{ij}}{RT} \cdot \left(C_{pi} - \frac{5}{2}R\right)}{1 + \sum_{\substack{j=2 \\ j\neq i}}^{\mu} \frac{D_{ii}}{D_{ij}} \cdot \frac{X_i}{X_j}} \quad (4)$$

With
$$C_{pi} = \frac{\partial}{\partial T}\left(\frac{5}{2}RT + RT^2 \frac{\partial \log(Q_{int}^i)}{\partial T}\right) \quad (5)$$

Where R is the perfect gas constant, Cpi the specific heat capacity of ith chemical specie, T the temperature and Q_{int}^i the internal partition function of ith specie. The formulation of the thermal conductivity chemical reaction was developed by Butler and Brokaw [13, 14, 18] and is written as:

$$\lambda_{react} = -\frac{1}{RT^2} \frac{\begin{vmatrix} A_{11} & \dots & A_{1\mu} & \Delta H_1 \\ \dots & A_{ii} & \dots & \dots \\ A_{\mu 1} & \dots & A_{\mu\mu} & \Delta H_\mu \\ \Delta H_1 & \dots & \Delta H_\mu & 0 \end{vmatrix}}{\begin{vmatrix} A_{11} & \dots & A_{1\mu} \\ \dots & A_{ii} & \dots \\ A_{\mu 1} & \dots & A_{\mu\mu} \end{vmatrix}} \quad (6)$$

With
$$A_{ij} = A_{ji} = \sum_{k=1}^{\mu-1} \sum_{l=k+1}^{\mu} \left(\frac{RT}{PD_{kl}}\right) \cdot X_k X_l \cdot \left[\frac{a_{ik}}{X_k} - \frac{a_{il}}{X_l}\right]\left[\frac{a_{jk}}{X_k} - \frac{a_{jl}}{X_l}\right] \quad (7)$$

$$D_{ij} = \frac{2,628.10^{-2}}{P} \cdot \frac{T^{\frac{3}{2}}}{\overline{\Omega}_{ij}^{(1,1)}}\left(\frac{M_i + M_j}{2M_i M_j}\right)^{\frac{1}{2}} \quad (8)$$

i^{th} reaction can be written as:

$$\sum_{k=1}^{\nu} a_{ki} B^k = O \quad (9)$$

Where B^k is the symbol of the k chemical species. The μ reactions that we have to take into account must be linearly independent. For the ith reaction the enthalpy variation ΔH_i is given by:
$$\Delta H_i = \sum_{j=1}^{\nu} a_{ij} H_j \quad (10)$$

Where H_j is the specific enthalpy of the jth chemical species and P the pressure.

2.2) Electrical conductivity coefficient

The electrical conductivity σ at thermal equilibrium is obtained using the third-order approximation of the Chapman-Enskog method [14, 18]:

$$\sigma = \frac{3e^2}{2}n_1^2 \sqrt{\frac{2\pi}{m_1 kT}} \frac{\begin{vmatrix} q^{11} & q^{12} \\ q^{12} & q^{22} \end{vmatrix}}{\begin{vmatrix} q^{00} & q^{01} & q^{02} \\ q^{01} & q^{11} & q^{12} \\ q^{02} & q^{12} & q^{22} \end{vmatrix}} \quad (11)$$

Where e is the electronic charge, n_1 the electrons density number, k the Boltzmann constant, m_1 mass of an electron and T is the temperature. The parameters q^{ij} are a function of density and collisions integral are given in [14].

2.3) Coefficient of viscosity

The viscosity can be considered mainly due to the heavy chemical species because of the mass ratio between electrons and heavy chemical species. We use the formulation given in [13]:

$$\eta = -\frac{\begin{vmatrix} H_{11} & \dots & H_{1\mu} & X_1 \\ \dots & \dots & \dots & \dots \\ H_{1\mu} & \dots & H_{\mu\mu} & X_\mu \\ X_1 & \dots & X_\mu & 0 \end{vmatrix}}{\begin{vmatrix} H_{11} & \dots & H_{1\mu} \\ \dots & \dots & \dots \\ H_{1\mu} & \dots & H_{\mu\mu} \end{vmatrix}} \quad (12)$$

Where H_{ij} are function of collision integrals, molar mass and molar fraction.

3) Choice of the potential and collision integrals
3.1) Neutral - neutral interactions
Many type of potential have been suggested to describe the interaction between two neutral particles [12]. In this paper we choose to use (12 - 6) Lennard-Jones potential for interaction between two atoms and deduce from simple combining rules the Lennard-Jones potentials for the other interaction for other neutral species. We have used the values found in the works of André and al. [14]. In table 1, we summarize the values of the Lennard-Jones parameters used in the case of the interaction between two neutral atoms simple combining rules [12].When the parameters of (12-6) Lennard-Jones potentials are determined, the average cross sections are determined from the table of Klein and Smith [12, 14, 18, 24].

Table 1: Parameters of Lennard -Jones potentials used in the present work.

Species		(σ) (Å)	(ℇ) (K/particle)	References
H	H	2.4	40	[12]
O	O	3.050	106.700	[11][19]
N	N	3.298	71.400	[11] [12]

3.2) Electrons - neutral interactions
For electrons-neutral collision, the average cross sections $\overline{Q}_{ij}^{(1,s)}$ with s included between 1 and 5, are calculated by [14]:

$$\overline{Q}_{ij}^{(1,s)} = a_1 \ln(T) + a_2 + a_3 T + \frac{a_4}{T} + a_5 T^{-2} + a_6 T^{-3} + a_7 T^{-4} \quad (13)$$

T is the temperature, the fitting coefficients a_i are taken in [14]. For missing data we use the rigid spheres approximations [24].

3.3) Ion - neutral interactions
For $M - M^+$ interactions, the resonant charge exchange is a dominant process to determine the average collision integrals [11,14,18, 23, 25]:

$$\overline{\Omega}_{M-M^+}^{(l,s)} = \frac{1}{\pi}\left\{\begin{array}{l} A^2 - AB\ln(4R) + \left(\frac{B\ln(4R)}{2}\right)^2 + \frac{B\xi}{2}\left(B\ln(4R) - 2A\right) + \\ \frac{B^2}{4}\left(\frac{\pi^2}{6} - \sum_{n=1}^{s+1}\frac{1}{n^2} + \xi^2\right) + \frac{B}{2}\left[B(\ln(4R)+\xi) - 2A\right]\ln\left(\frac{T}{M}\right) + \left(\frac{B}{2}\ln\left(\frac{T}{M}\right)\right)^2 \end{array}\right\} \quad (14)$$

R is the perfect gas constant, $\xi = \sum_{n=1}^{s+1}\frac{1}{n} - \overline{\gamma}$ with $\overline{\gamma}$ the Euler constant ($\overline{\gamma}$ =0.577216) and M the atomic weight (gmol^{-1}) of the atomic species M. In table 2, we give the values of the parameters A and B that we used in our calculations. For the other collisions

between neutral and charged particles, we considered them as elastic and that the charge particle engenders a dipole in the neutral particles during the collision. From the paper of Kihara and al, we obtain the cross section by the formula [14,18, 23, 25]:

$$\overline{\Omega}_{ij}^{(l,s)} = \frac{4(l+1)}{(s+1)!\left(2l+1-(-l)^l\right)}\sqrt{\frac{4}{kT}}\sqrt{\frac{\alpha Z\ell^2}{4\pi\varepsilon_0}}\Gamma\left(s+\frac{3}{2}\right)A_4^{(l)} \quad (15)$$

$A_4^{(l)}$ are parameters given in [18]. The polarisabilities α of neutral particle that we use in our calculation are given in [11, 12, 14, 19].

Table 2: Parameters A and B characterized resonant charge exchange used in the present work.

Species		A	B	References
H	H$^+$	28.69	1.3	[12] [14]
O	O$^+$	19.5	0.832	[12] [14]
N	N$^+$	26.61	1.27	[12] [14]
O$_2$	O$_2^+$	24.05	1.132	[14]
NO	NO$^+$	23.61	1.095	[14]
N$_2$	N$_2^+$	24.5	1.032	[14]

3.4) Charged - charged interactions

The average cross section for interactions between charged species has been calculated from coulomb potential [1, 5, 12, 14, 25]. Using the expression from transport sections efficacies of Liboff, Devoto [1, 5] established the following formulas:

$$\overline{Q}^{(1,s)} = \frac{4\pi}{s(s+1)}b_0^2\left[\ln\left(\frac{2\lambda_D}{b_0}\right)-\frac{1}{2}-2\gamma+\psi(s)\right] \quad (16)$$

$$\overline{Q}^{(2,s)} = \frac{12\pi}{s(s+1)}b_0^2\left[\ln\left(\frac{2\lambda_D}{b_0}\right)-\frac{1}{2}-2\gamma+\psi(s)\right] \quad (17)$$

Where $\psi(s) = \sum_{n=1}^{s-1}\frac{1}{n}$; $\psi(1) = 0$, $b_0 = \frac{Z_iZ_je^2}{2kT}$.

The Debye length taken in to account the presence of electrons and ions is given by [26]:

$$\lambda_D = \left(\varepsilon_0 R\sum_{i=1}^{N}\frac{T}{q_i^2 n_i}\right) \quad (18)$$

Where ε_0 is the vacuum permittivity and q_i the electrical charge of the ith species.

4) Results and discussions

4.1) Test of calculation program

In this section, we have tested our calculation program by comparing our results with a well-know values of dry air of the work of P. Fauchais and al [27]. On figures 1, 2 and 3, we respectively compare the total thermal conductivity, the electrical conductivity and the dynamical viscosity of our work with those of P. Fauchais. Figure 1 shows that our results of total thermal conductivity and those of P. Fauchais and al are in good agreement with a less than 20% maximum variation around 4500K, 7500K and 9000K. The electrical conductivity in figure 2 is in good agreement in all the range of temperature. For dynamical viscosity, the maximum discrepancy around 10700K is less than 10%. The different discrepancies in total thermal conductivity and dynamical viscosity can be due to the results of equilibrium composition and the integral collisions used in the transport coefficients calculation.
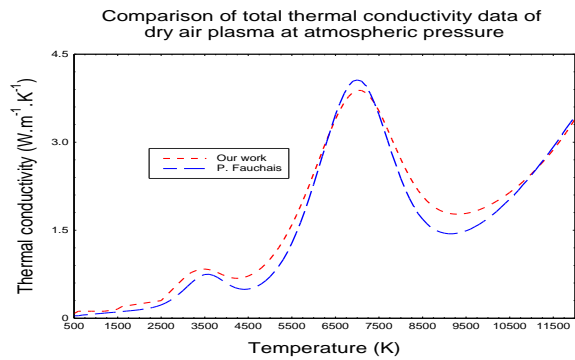

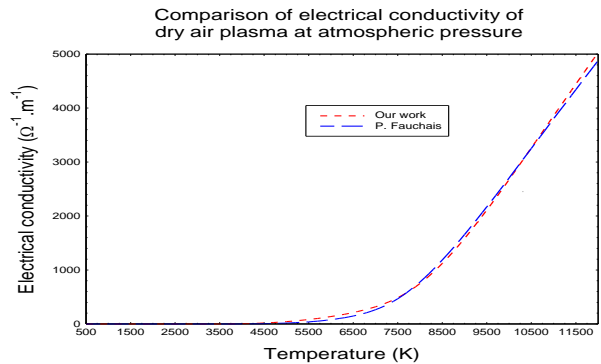**Figure 1**: Comparison of thermal conductivity of our work with the one of P. Fauchais and al.

Figure 2: Comparison of electrical conductivity of our work with the one of P. Fauchais and al.
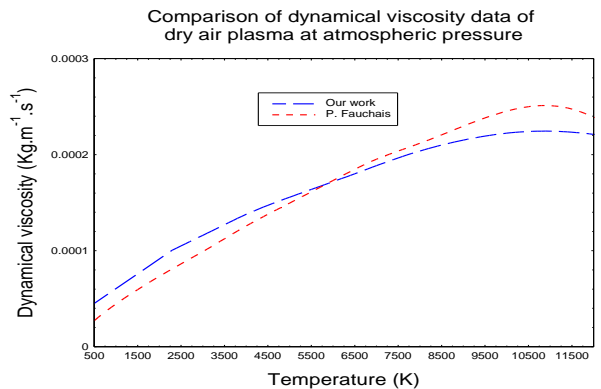

Figure 3: Comparison of dynamical viscosity of our work with the one of P. Fauchais and al.

4.2) Influence of water vapor's rate on transport coefficients

In figure 4, we have plotted the total thermal conductivity for different proportions of water vapor. Each curve exhibits two peaks: the first one around 3500 K is related to O$_2$ and H$_2$O dissociation, the second one around 7500 K to N$_2$ dissociation. The peaks related to ionization reactions occur at temperatures above 12000 K [1], which is out of our temperature range. The peak which appears around 3500 K, increases when the rate of water vapor increases in the mixture and the one around 7500 K decreases when the rate of water vapor increases in the mixture because the increase of water vapor's rate in the mixture contribute to the increase of the density of chemical species which dissociates at 3500 K (H$_2$O) and decreases the chemical species which dissociates around 7500 K (N$_2$). The peak around 3500 K is very sensitive to the variation of the rate of water vapor. For temperatures below 6000 K and above 8000 K, the total thermal conductivity increases with the rate of water vapor in the plasma, and for temperatures between 6000 K and 8000 K, the total

thermal conductivity decreases when the rate of water vapor increases in the medium.

The researches undertaken by various authors Hertz [1, 5], Vacquié [1, 5] have showed that thermal conductivity has a very significant role on the time constant of arc (τ). Consequently the shape of thermal conductivity curve gives important information on the performance of the gas used for the electrical arc extinction [1]. From the study of several gases, Hertz [1, 5] proposes an empirical relation linking the arc time-constant (τ) to the maximum value of the reaction thermal conductivity component [1, 5, 28] of the gas: $\tau.\lambda_{react}^{\max} = C^{te}$. This relation shows the role of the reaction thermal conductivity component in the velocity of electrical arc extinction. The more the reaction thermal conductivity is high, the more the electrical arc extinct rapidly. So, the shape of the curve shows that the increase of water vapor in the mixture can be interesting for electrical arc extinction.

In figure 5, we have plotted the electrical conductivity versus temperature for different proportions of water vapor. The electrical conductivity increases with temperature because the density of electrons increases when the temperature increases in the medium. The electrical conductivity decreases when the rate of water vapor increases in the mixture, because the increase of the rate of water in the mixture decreases the density of chemical species NO which are responsible by ionization of the production of electrons in low temperatures. That can be interesting for a good performance of the circuit breaker which uses this kind of gas. The shape of the curve shows that the electrical conductivity increases with the rate of water vapor in high temperature [1].

The dynamical viscosity of the studied plasmas is given versus temperature on figure 6. We obtain the shape of curves found in the literature. The results show an increase followed by a decrease versus temperature. The dynamical viscosity increases with temperature and reached its maximum value around 10000 K, which characterizes the transition between neutral or partially ionized plasma towards totally ionized plasma [13]. The decrease is due to the apparition of electrons and ionized chemical species [14] in the plasma. The dynamical viscosity decreases when the rate of water vapor increase in the mixture, because the molar weight of water molecule (H_2O) is inferior to that of nitrogen molecule (N_2). We noticed a rapid increasing of the dynamical viscosity around 3500 K which correspond to the temperature of dissociation of water molecule (H_2O).
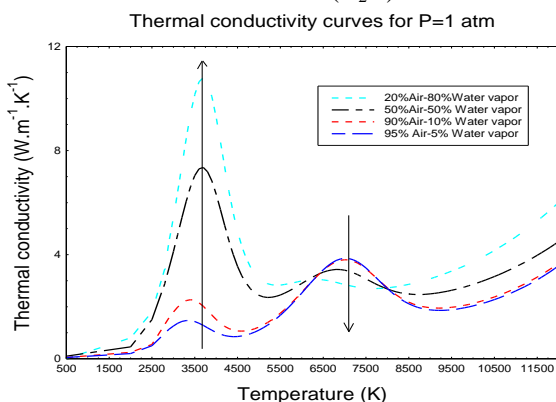

Figure 4: The total thermal conductivity versus temperature for the four mixture plasmas.
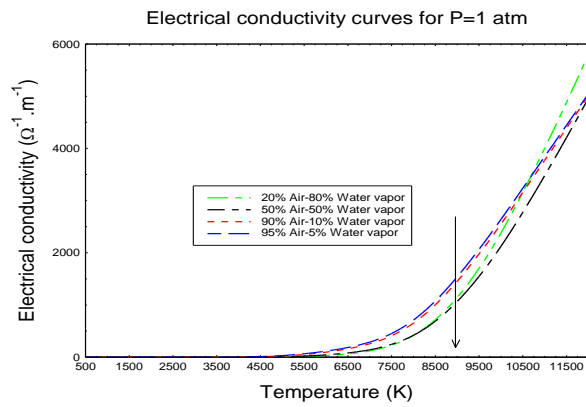

Figure 5: The electrical conductivity versus temperature for the four mixture plasmas.
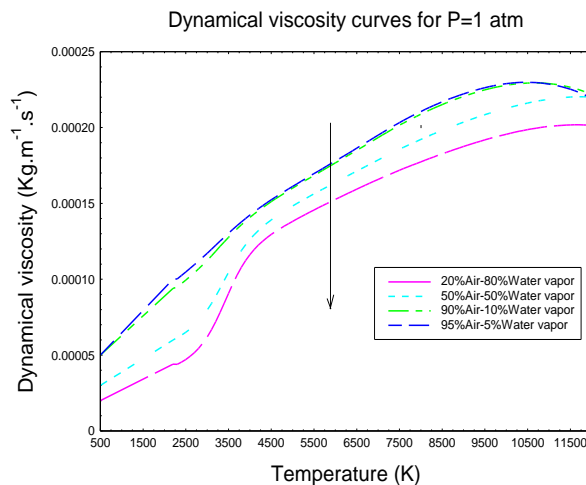

Figure 6: The dynamical viscosity versus temperature for the four mixture plasmas.

5) Conclusion

We have presented the results of the transport coefficients of the plasma formed of air-water vapor mixtures. This study completes the one of Kagoné and al [1] to have a database on the range of temperatures from 500 K to 30000 K for the modeling of plasma formed by air- water vapor mixtures. The results of thermal conductivity, electrical conductivity and dynamical viscosity versus temperature are presented and discuss. For temperatures less than 6000 K and above 8000 K, the thermal conductivity increases with the rate of water vapor. The peak around 3500 K is very sensitive to the variation of the rate of water vapor. The electrical conductivity decreases when the rate of water vapor increases at low temperatures. The dynamical conductivity decreases when the rate of water vapor increases in the medium. According to the empirical formula [1, 5, 28] $\tau.\lambda_{react}^{\max} = C^{te}$ and the decrease of electrical conductivity, the increase of the rate of water vapor can be interesting for the improvement of the performance of circuit breaker using this kind of gas.

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